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Biological activity, chemical profiling and molecular docking of tissue extracts of the sea snail *Trochus erithreus*

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SUPPLEMENTARY MATERIAL

Table 1S. Chemical compositions of *Te*-Acetone extract

No.	R_t	Area%[a]	M.W.	M.F.	Identified compounds	Class/Category
1	5.11	1.88	86	$C_5H_{10}O$	Propane, 2-(ethenyloxy)	Aliphatic ether
2	9.24	0.70	136	$C_{10}H_{16}$	l-Limonene	Monoterpenes
3	19.61	1.01	226	$C_{14}H_{26}O_2$	Z9-Dodecenyl acetate	Fatty alcohol esters
4	20.87	7.89	204	$C_{15}H_{24}$	(E)-α-Farnesene	Sesquiterpenoids

5	21.48	0.57	204	$C_{15}H_{24}$	Germacrene D	Sesquiterpenoids
6	22.12	0.55	154	$C_{10}H_{18}O$	Cis-Myrtanol	Bicyclic monoterpenoids
7	22.40	0.95	206	$C_{16}H_{14}$	15-methyltricyclo[6.5.2(13,14).0(7,15)] pentadeca-1,3,5,7,9,11,13-heptene	Cyclic alkane derivatives
8	23.48	1.17	182	$C_{12}H_{22}O$	3-Dodecen-1-al	Medium-chain aldehydes
9	23.94	0.59	200	$C_{13}H_{28}O$	Tridecanol	Long-chain fatty alcohol
10	25.22	0.52	204	$C_{15}H_{24}$	α-copaene	Sesquiterpenoids
11	25.50	2.99	238	$C_{15}H_{26}O_2$	α-Bisabolol-oxide-B	Sesquiterpenoids
12	25.77	1.01	252	$C_{17}H_{32}O$	8-Hexadecenal, 14-methyl, (Z)	Fatty aldehydes
13	26.14	2.92	236	$C_{15}H_{24}O_2$	Bisabolone oxide	Sesquiterpenoids
14	27.19	0.84	184	$C_{14}H_{16}$	Chamazulene	Sesquiterpenoids
15	27.52	24.63	238	$C_{15}H_{26}O_2$	Bisabolol oxide A	Sesquiterpenoids
16	29.43	1.73	146	C10H10O	Methylcinnamic aldehyde	Cinnamaldehydes
17	29.81	1.64	226	$C_{15}H_{14}S$	trans-Cinnamyl phenyl sulfide	Cinnamaldehydes derivatives
18	30.34	1.32	200	$C_{13}H_{12}O_2$	1,6-Dioxaspiro[4.4]non-3-ene,2-(2,4-hexadiynylidene)	Alkyne derivatives
19	30.96	1.47	270	$C_{17}H_{34}O_2$	Pentadecanoic acid, 14-methyl, methyl ester	Fatty acid esters
20	31.77	2.89	130	$C_{10}H_{10}$	Cycloprop[a]indene, 1,1a,6,6a-tetrahydro	Tetralins
21	31.89	4.21	210	$C_{14}H_{14}N_2$	2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)] propanenitrile	Naphthalene derivatives
22	32.08	5.41	156	$C_{12}H_{12}$	Tricyclo[8.2.0.0(2,5)]dodeca-3,6,8,11-tetraene	Annulenes
23	32.23	2.46	284	$C_{18}H_{36}O_2$	Hexadecanoic acid, ethyl ester	Fatty acid esters
24	33.62	0.84	156	$C_{11}H_8O$	Benzofulvene-8-carboxyldehyde	Aromatic aldehyde

Table 1S *Continue*

No.	R_t	Area%[a]	M.W.	M.F.	Identified compounds	Class/Category
25	33.89	1.71	242	$C_{16}H_{34}O$	1-Hexadecanol	Fatty alcohol
26	34.09	3.47	294	$C_{19}H_{34}O_2$	9,12-Octadecadienoic acid, methyl ester	Fatty acid esters
27	34.19	1.68	296	$C_{19}H_{36}O_2$	9-Octadecenoic acid, methyl ester	Fatty acid esters

28	35.48	1.59	161	$C_{10}H_{11}NO$	N-Allylbenzamide	Benzamides
29	35.80	2.60	312	$C_{20}H_{40}O_2$	Octadecanoic acid, ethyl ester	Fatty acid esters
30	36.40	0.57	280	$C_{15}H_{20}O_5$	Tetraneurin A diol	Alcoholic compounds
31	36.87	0.78	160	$C_{12}H_{16}$	Benzene, (1,3-dimethyl-3-butenyl)	Benzene and substituted derivatives
32	36.92	1.40	176	$C_{13}H_{20}$	Benzene, (1-methylhexyl)	Benzene and substituted derivatives
33	37.21	0.88	206	$C_{16}H_{14}$	Benzene, 1,1'-(1,3-butadiene-1,4-diyl)bis	Diphenyl diene derivatives
34	37.80	0.79	168	$C_{11}H_{20}O$	trans-Undec-4-enal	Medium-chain aldehydes
35	37.89	0.61	282	$C_{18}H_{34}O_2$	9-Octadecenoic acid (Z)	Fatty acids
36	38.50	3.03	210	$C_{14}H_{26}O$	3-Tetradecyn-1-ol	Unsaturated fatty alcohol
37	41.55	1.62	390	$C_{24}H_{38}O_4$	1,2-Benzenedicarboxylic acid, diisooctyl ester	Benzoic acid esters
38	45.46	0.58	192	$C_{14}H_{24}$	1,5,9-Undecatriene, 2,6,10-trimethyl, (Z)	Acyclic monoterpenoids
39	46.07	0.62	214	$C_{14}H_{30}O$	Hexyl octyl ether	Long chain ether
40	46.46	0.77	446	$C_{28}H_{46}O_4$	1,2-Benzenedicarboxylic acid, bis(8-methylnonyl) ester	Benzoic acid esters
41	46.65	0.71	368	$C_{22}H_{40}O_4$	Cyclopropanedecanoic acid, à-(acetyloxy)-2-hexyl, methyl ester	Fatty acid methyl esters
42	46.88	0.84	446	$C_{28}H_{46}O_4$	1,2-Benzenedicarboxylic acid, diisodecyl ester	Benzoic acid esters
43	47.06	0.80	446	$C_{28}H_{46}O_4$	Phthalic acid, didecyl ester	Benzoic acid esters
44	47.27	0.64	418	$C_{26}H_{42}O_4$	Phthalic acid, decyloct-3-ylester	Benzoic acid esters
45	47.68	0.65	292	$C_{19}H_{32}O_2$	6,9,12-Octadecatrienoic acid, methyl ester	Fatty acid methyl esters
		T% 96.53				

Rt: Retention time; **M.W.:** Molecular weight; **M.F.:** Molecular formula.

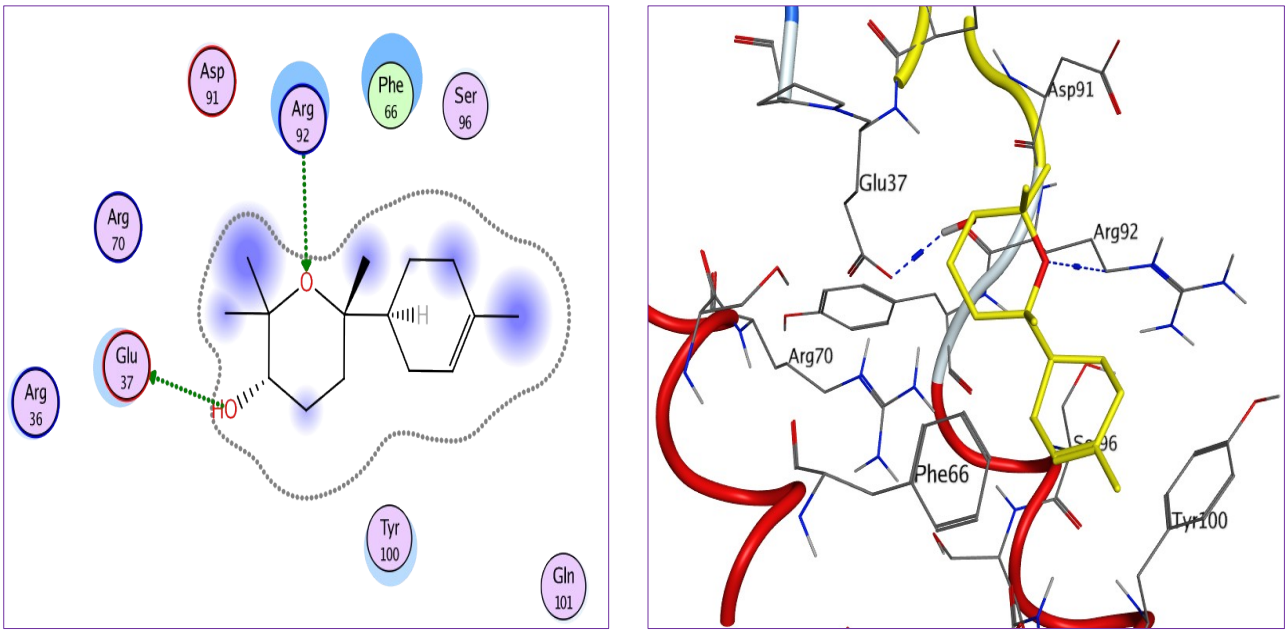

Fig. 1S. The two-dimensional and three-dimensional suggested binding modes of Bisabolol oxide within the binding pocket of TMK (PDB: 4QGG)

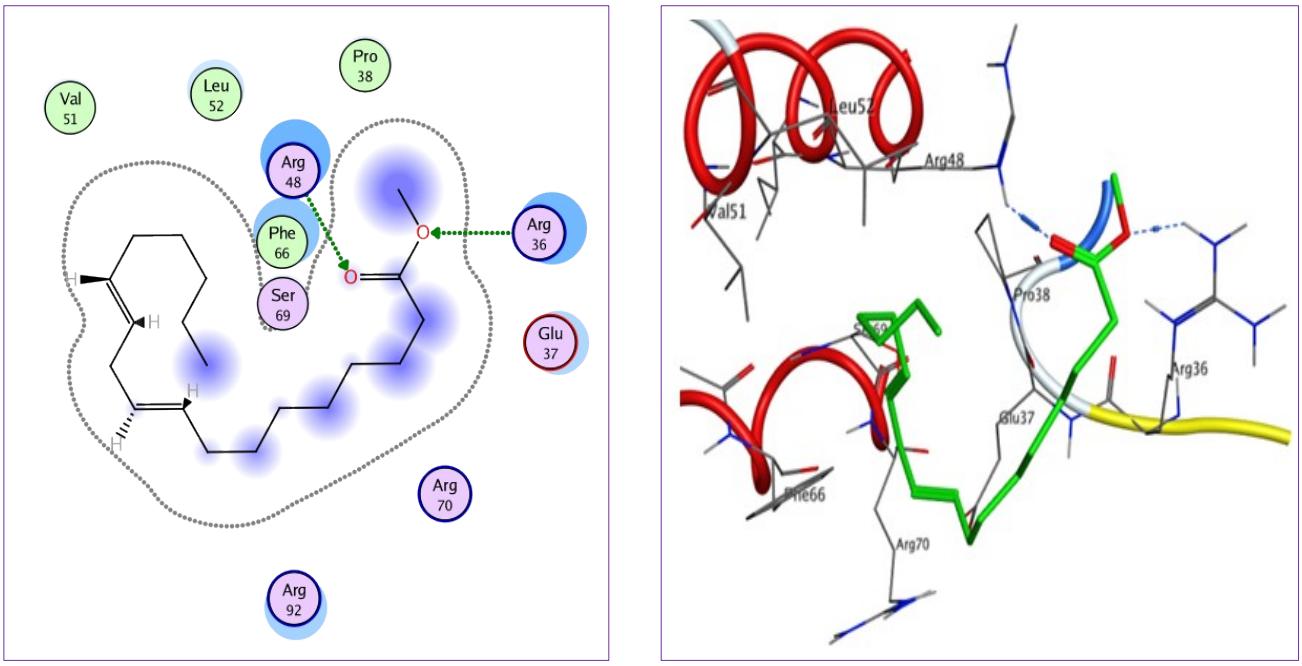

Fig. 2S. The two-dimensional and three-dimensional suggested binding modes of 9,12-Octadecadienoic acid, methyl ester within the binding pocket of TMK (PDB: 4QGG)

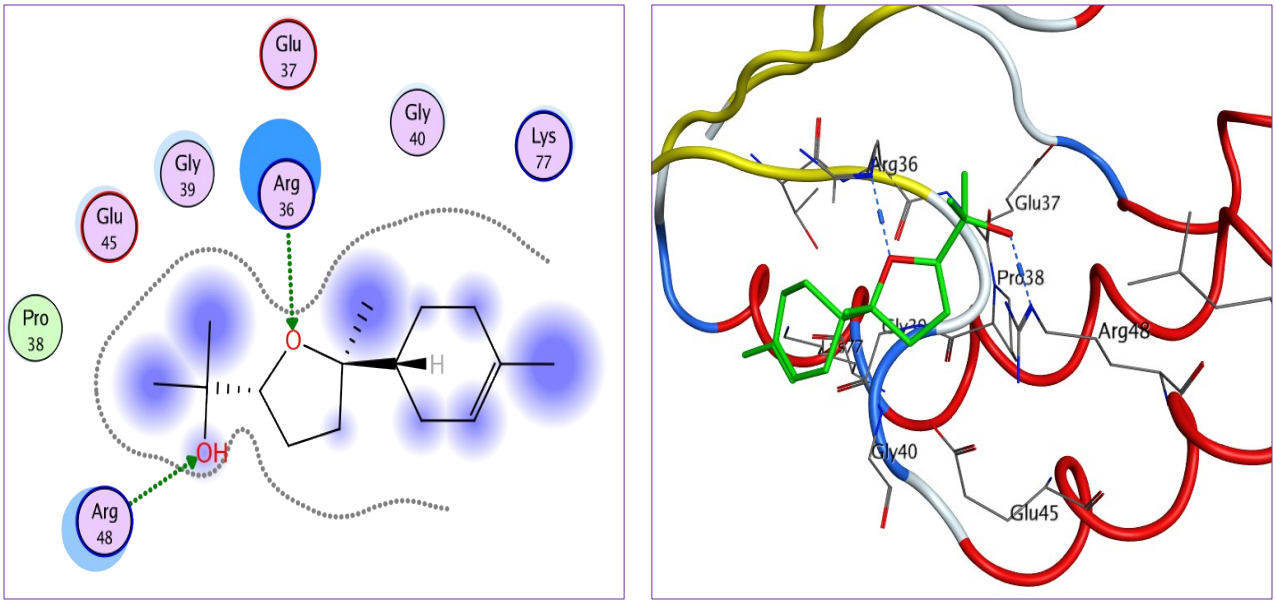

Fig. 3S. The two-dimensional and three-dimensional suggested binding modes of α-Bisabolol-oxide-B within the binding pocket of TMK (PDB: 4QGG)

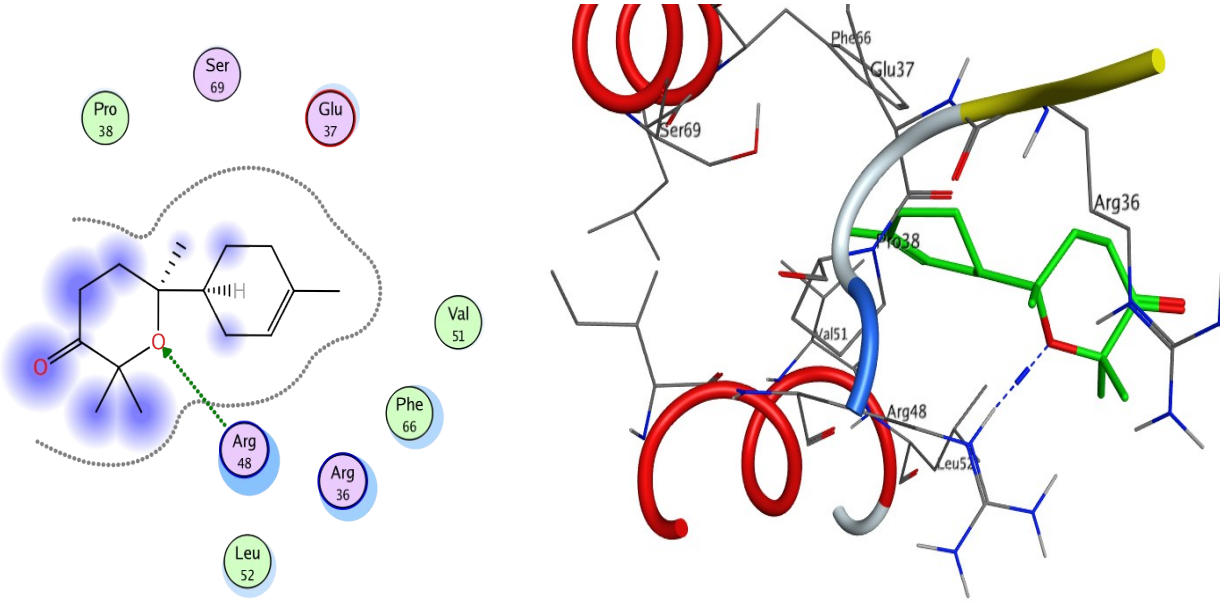

Fig. 4S. The two-dimensional and three-dimensional suggested binding modes of Bisabolone oxide within the binding pocket of TMK (PDB: 4QGG)

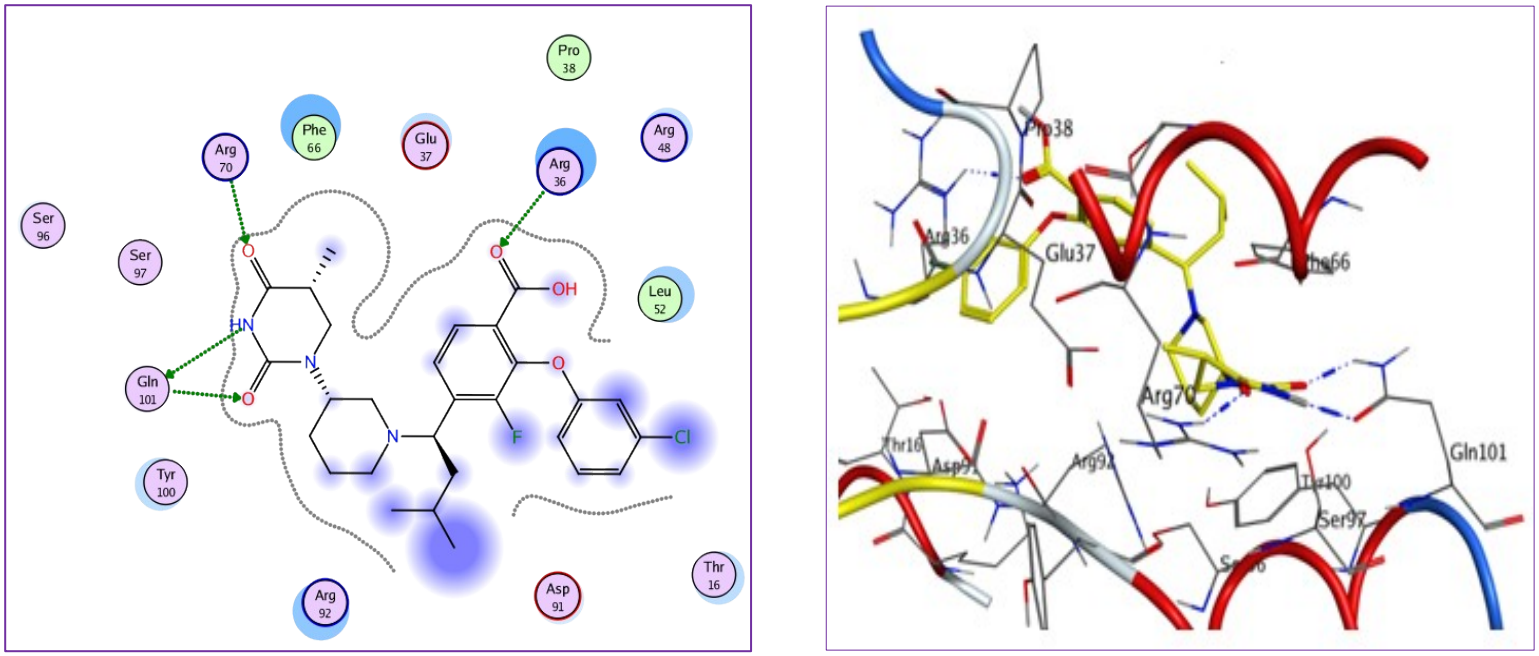

Fig. 5S. The two-dimensional and three-dimensional suggested binding modes of redocked ligand within the binding pocket of TMK (PDB: 4QGG)

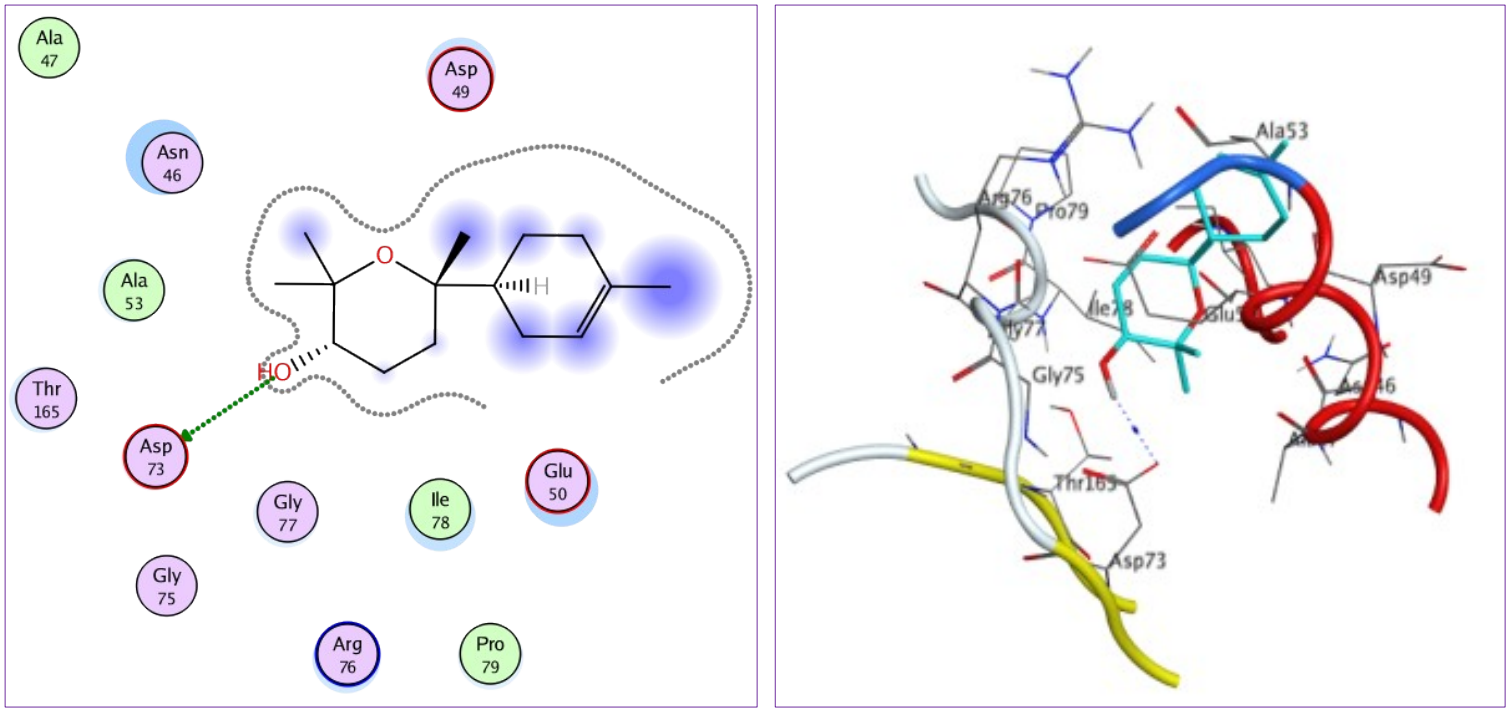

Fig. 6S. The two-dimensional and three-dimensional suggested binding modes of Bisabolol oxide A within the binding pocket of DNA gyrase B (PDB: 6F86).

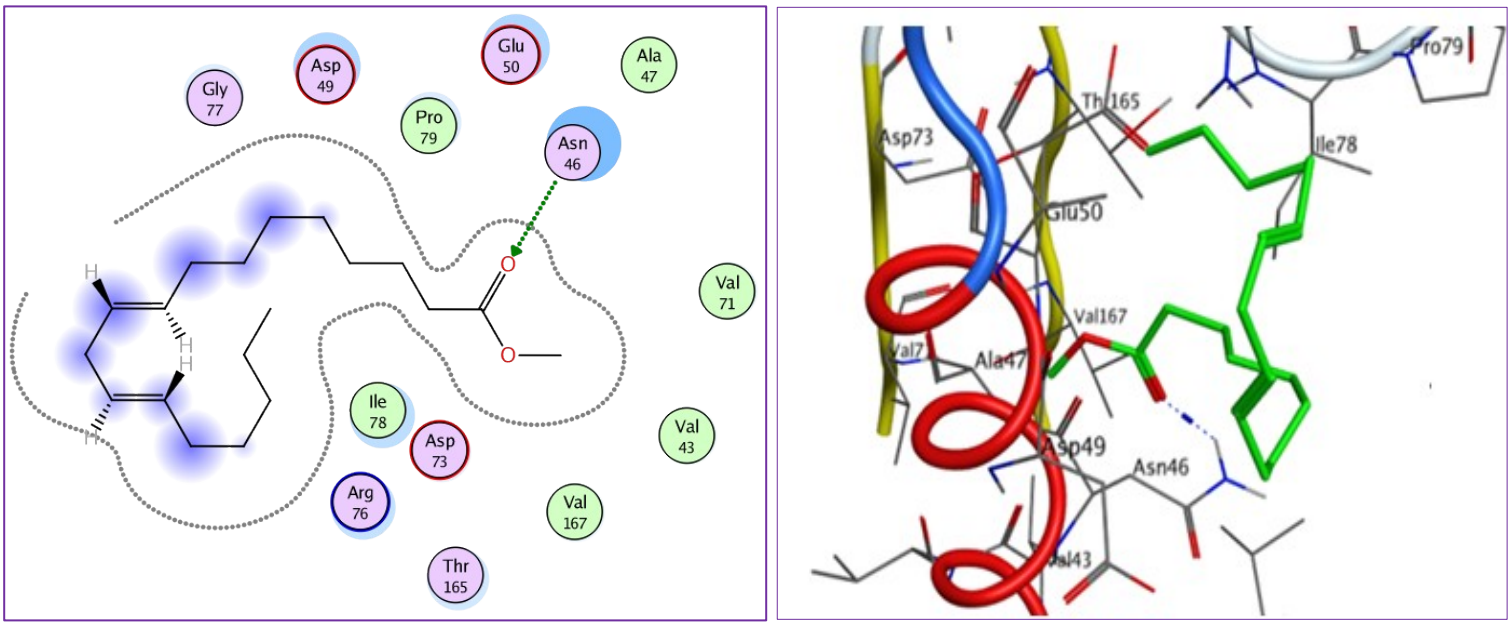

Fig. 7S. The two-dimensional and three-dimensional suggested binding modes of 9,12-Octadecadienoic acid, methyl ester within the binding pocket of DNA gyrase B (PDB: 6F86).

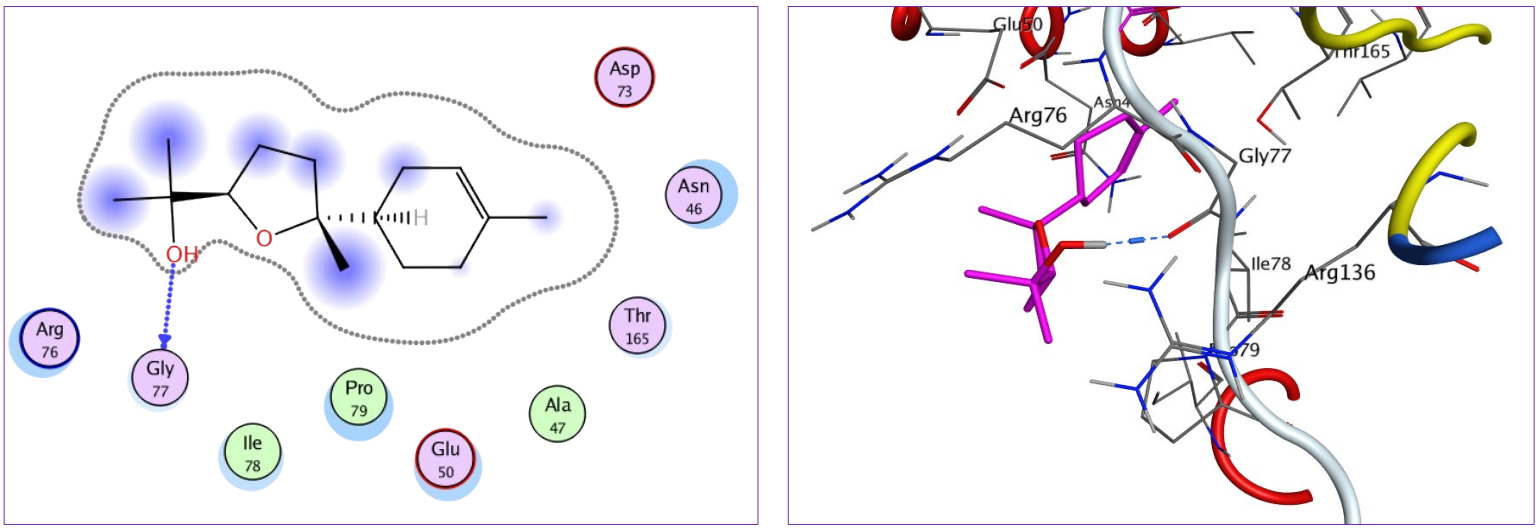

Fig. 8S. The two-dimensional and three-dimensional suggested binding modes of α-Bisabolol-oxide-B within the binding pocket of DNA gyrase B (PDB: 6F86).

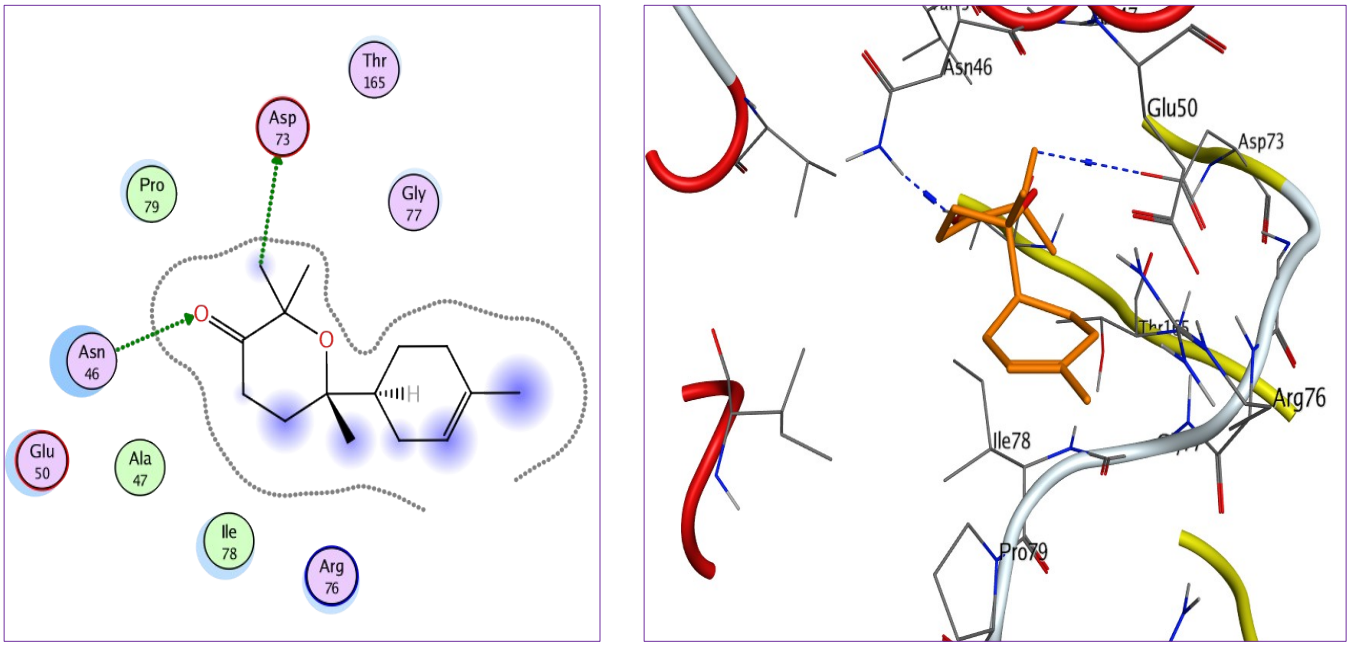

Fig. 9S. The two-dimensional and three-dimensional suggested binding modes of Bisabolone oxide within the binding pocket of DNA gyrase B (PDB: 6F86).

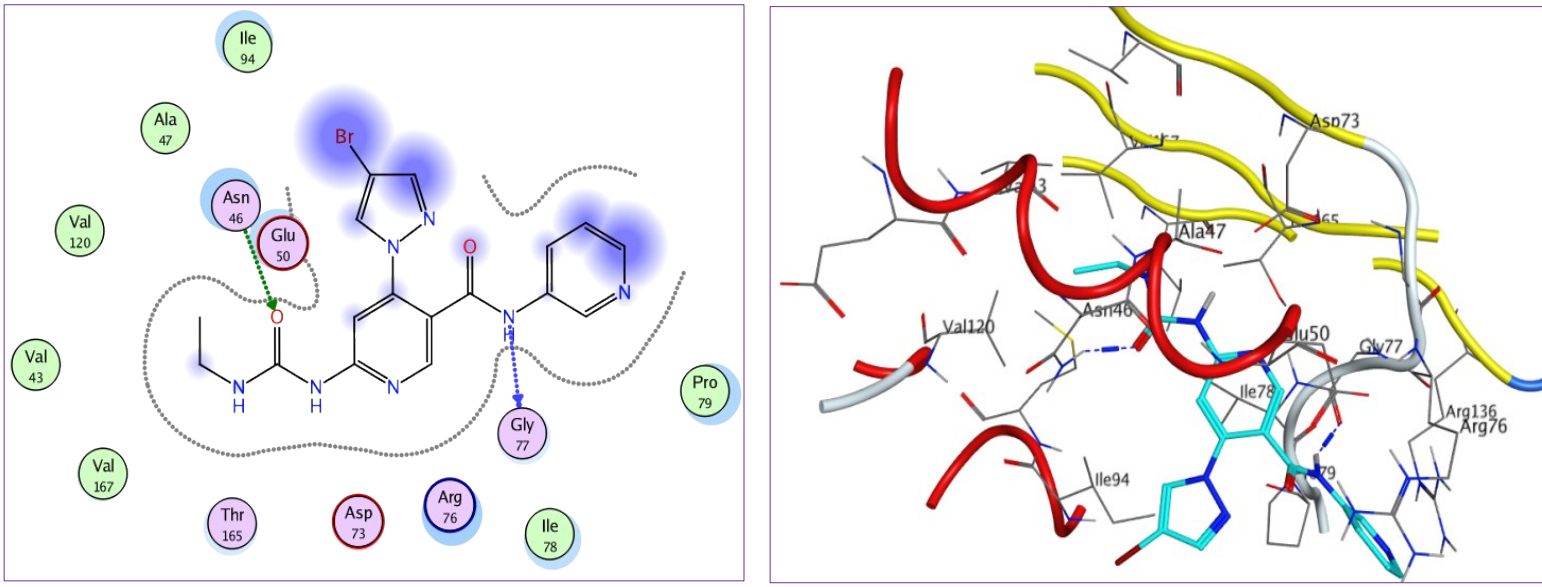

Fig. 10S. The two-dimensional and three-dimensional suggested binding modes of redocked ligand within the binding pocket of DNA gyrase B (PDB: 6F86).

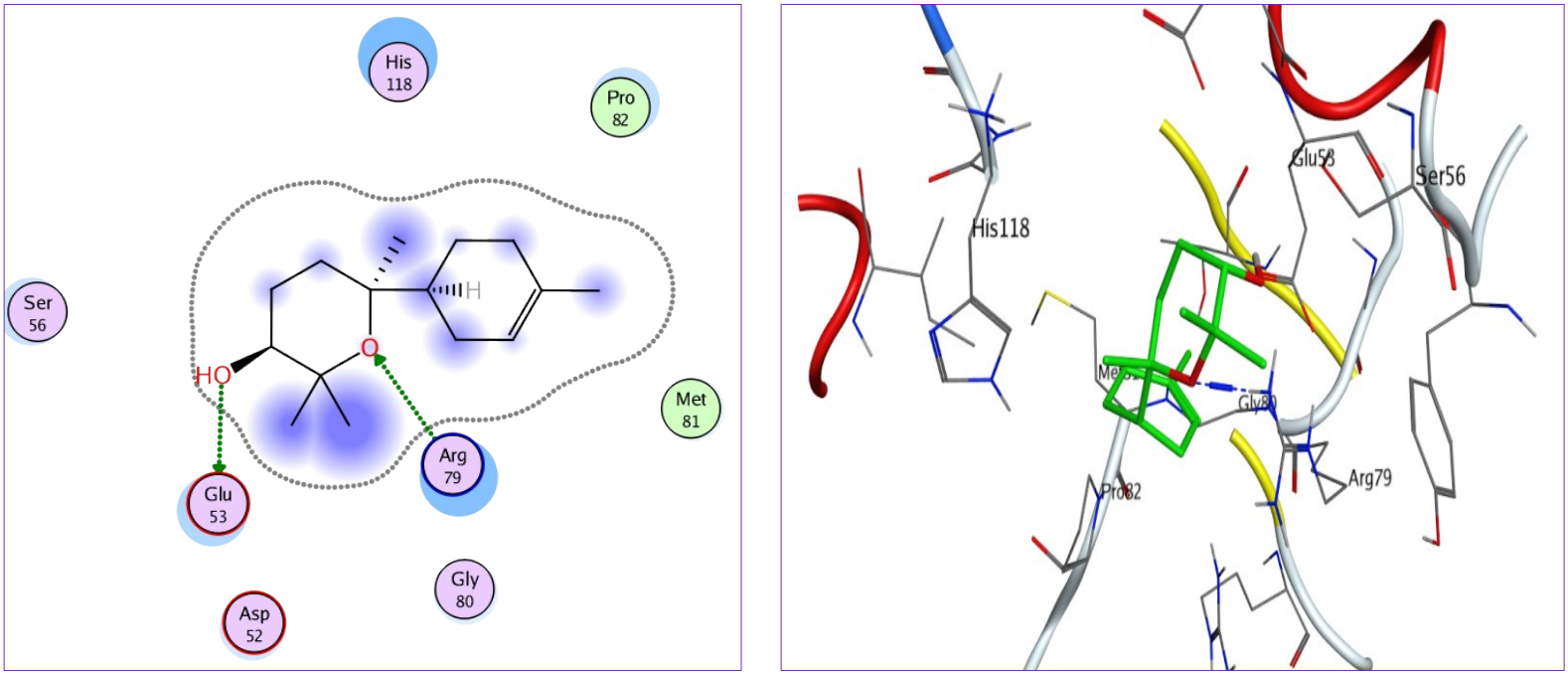

Fig. 11S. The two-dimensional and three-dimensional suggested binding modes of Bisabolol oxide A within the binding pocket of DNA topoisomerase IV subunit B (PDB: 4HZ5)

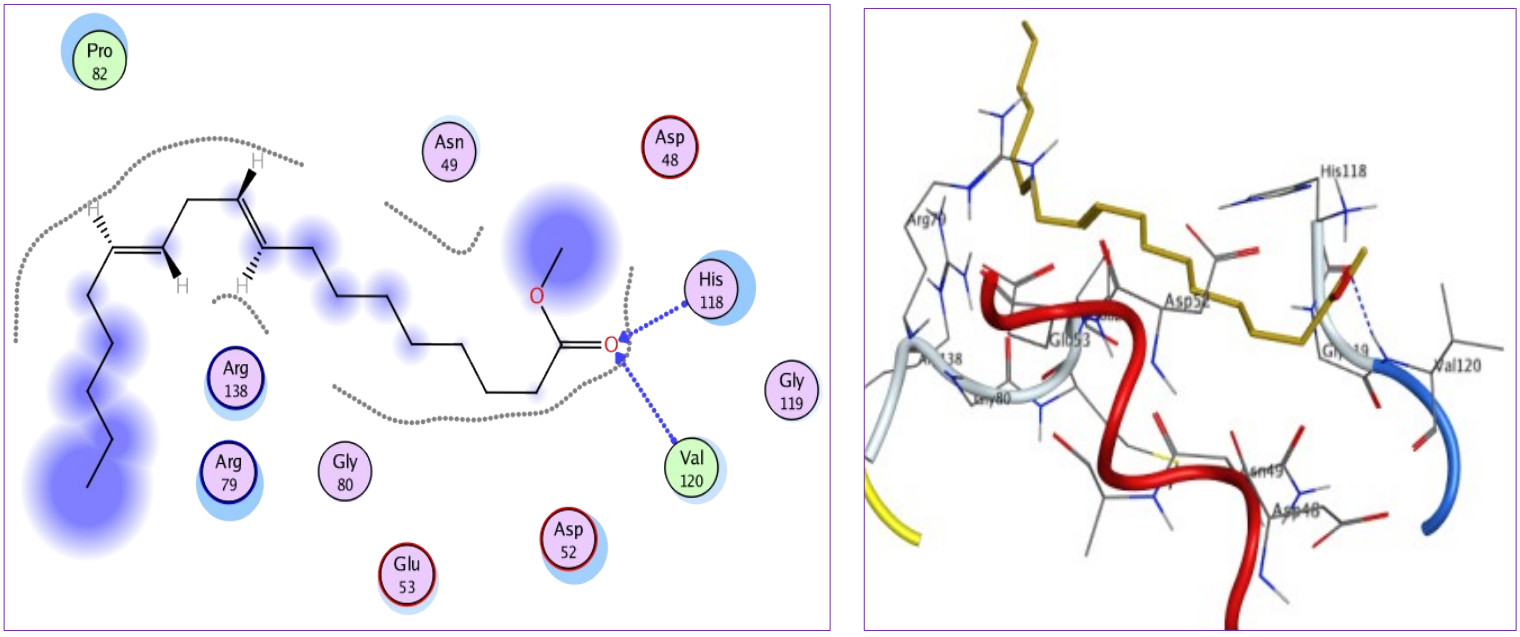

Fig. 12S. The two-dimensional and three-dimensional suggested binding modes of 9,12-Octadecadienoic acid, methyl ester within the binding pocket of DNA topoisomerase IV subunit B (PDB: 4HZ5).

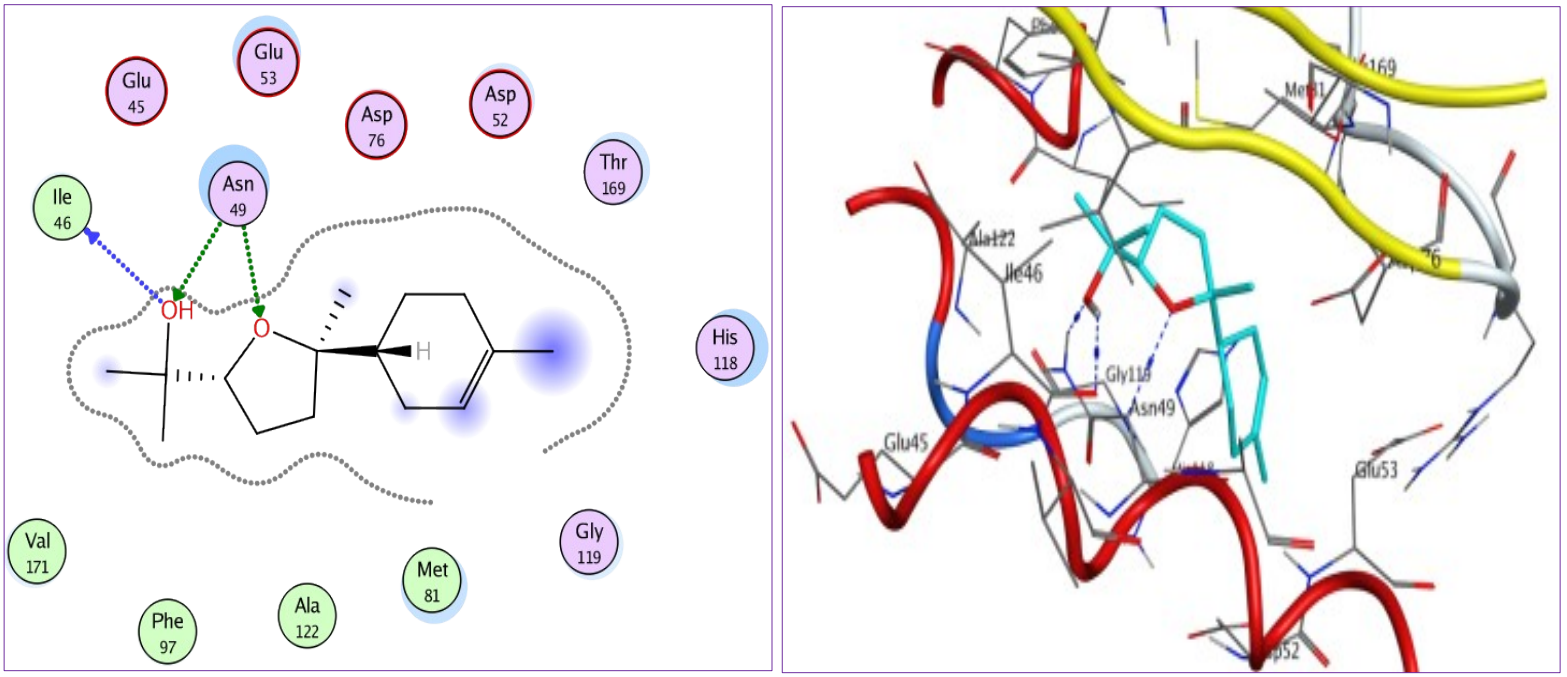

Fig. 13S. The two-dimensional and three-dimensional suggested binding modes of α-Bisabolol-oxide-B within the binding pocket of DNA topoisomerase IV subunit B (PDB: 4HZ5).

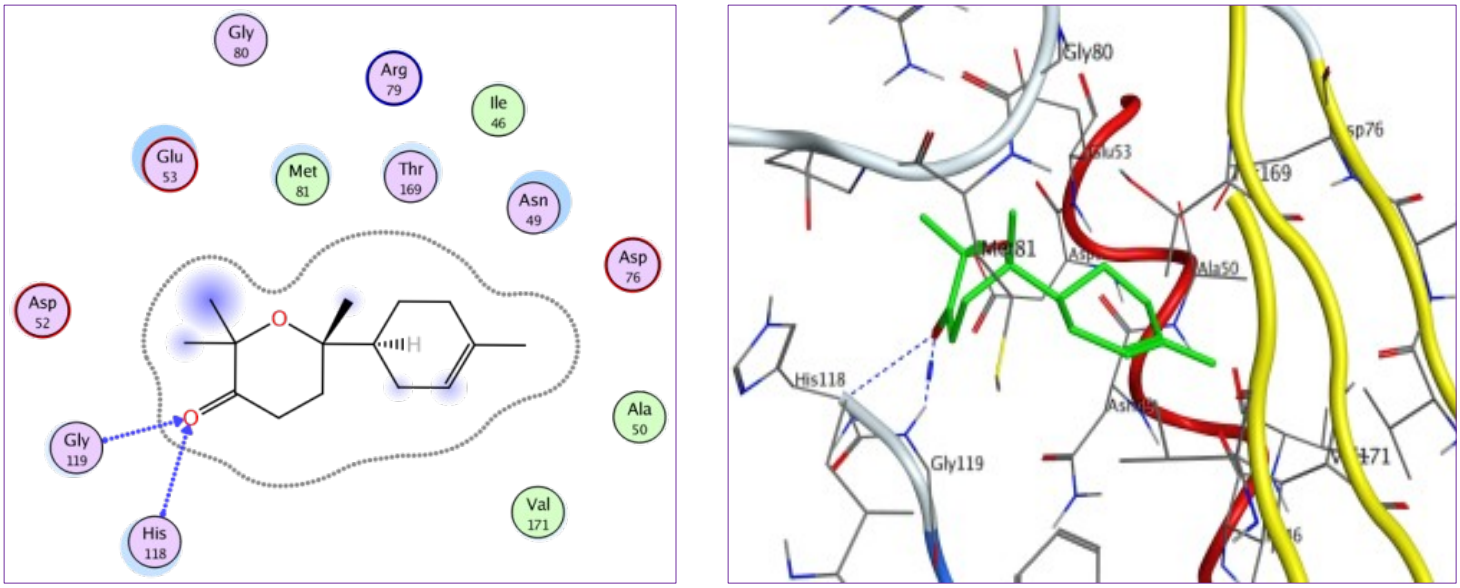

Fig. 14S. The two-dimensional and three-dimensional suggested binding modes of Bisabolone oxide within the binding pocket of DNA topoisomerase IV subunit B (PDB: 4HZ5).

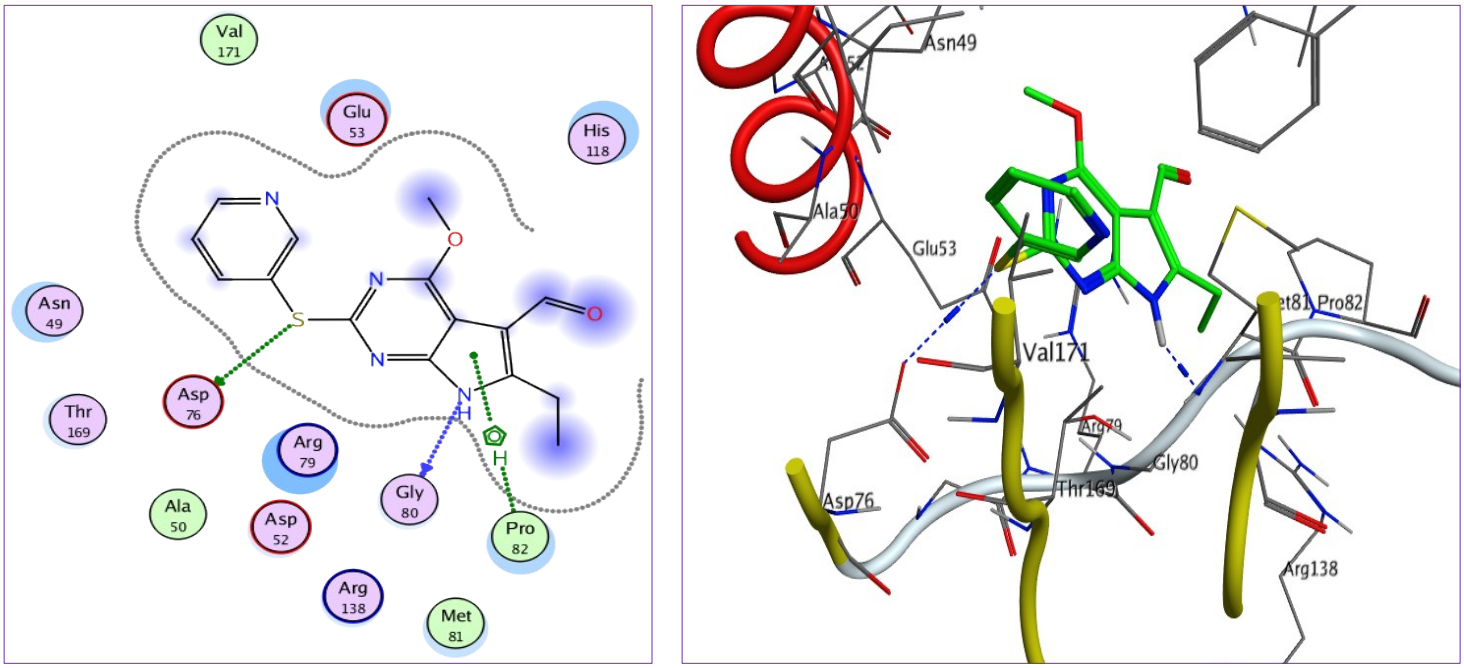

Fig. 15S. The two-dimensional and three-dimensional suggested binding modes of redocked ligand within the binding pocket of DNA topoisomerase IV subunit B (PDB: 4HZ5).